Lecture 12

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Load packages

```r
library(ggplot2)
library(dplyr)
```

```
##
## Attaching package: 'dplyr'
```

```
## The following objects are masked from 'package:stats':
##
##     filter, lag
```

```
## The following objects are masked from 'package:base':
##
##     intersect, setdiff, setequal, union
```

```r
library(broom)
Auto <- read.csv("Auto.csv",stringsAsFactors = FALSE)
Auto <- na.omit(Auto)
```

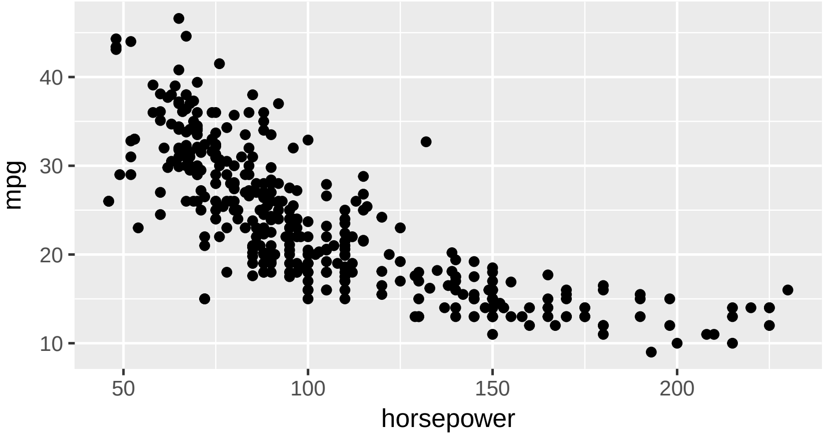
Cross-validation

- Reference: Chapter 5 of An Introduction to Statistical Learning with Applications in R Gareth James, Daniela Witten, Trevor Hastie and Robert Tibshirani

Example data

- Data on car mileage, engine size, car weight, for 392 cars made between 1970 and 1982.

```
ggplot(Auto,aes(x=horsepower,y=mpg)) + geom_point()
```



Predict mpg with polynomials in horsepower

```r
afit <- lm(mpg ~ horsepower + I(horsepower^2) + I(horsepower^3),
           data=Auto)
tidy(afit)
```

```
##              term      estimate    std.error  statistic      p.value
## 1     (Intercept)  6.068478e+01 4.563446e+00 13.2980167 1.649066e-33
## 2      horsepower -5.688501e-01 1.179222e-01 -4.8239460 2.025851e-06
## 3 I(horsepower^2)  2.079011e-03 9.479300e-04  2.1932117 2.888499e-02
## 4 I(horsepower^3) -2.146626e-06 2.378265e-06 -0.9026016 3.672973e-01
```

- Suggests we need only the linear and quadratic terms.

The validation method

- Randomly split the data into a “training” set and “test” set.
- Fit the model of each polynomial degree to the training set and use it to predict observations in the test set.
- Judge the fit of each model by the mean squared error in the test set, defined as $MSE = \frac{1}{n_{test}} \sum_i (y_i - \hat{y}_i)^2$, where n_{test} is the size of the test set.
- Choose the degree with the lowest MSE.

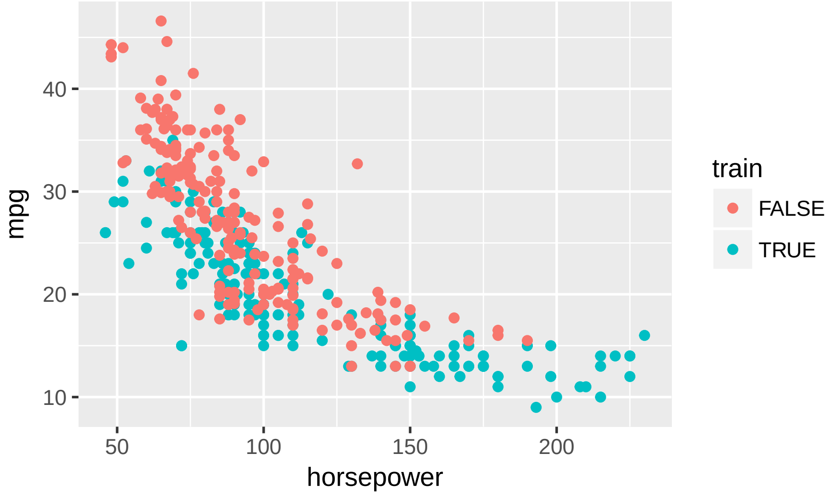
Split the data

- Several ways to do this.
  - E.G., permute the n rows and take the first $n/2$ to be the training set and the remaining $n/2$ to be the test set.

```r
n <- nrow(Auto)
inds <- 1:n
set.seed(42)
pAuto <- Auto[sample(inds),]
traininds <- 1:(n/2)
trainset <- pAuto[traininds,]
testset <- pAuto[-traininds,]
```

Split the data

```r
AutoT <- mutate(Auto, train = (inds %in% traininds))
ggplot(AutoT,aes(x=horsepower,y=mpg,color=train)) + geom_point()
```



Validation method on the Auto data

```r
validate <- function(dat,ndegrees) {
  n <- nrow(dat)
  pdat <- dat[sample(1:n),]
  traininds <- 1:(n/2)
  trainset <- pdat[traininds,]
  testset <- pdat[-traininds,]
  MSE <- vector(length=ndegrees)
  for(degree in 1:ndegrees) {
    fit <- lm(mpg ~ poly(horsepower,degree),data=trainset)
    ptest <- predict(fit,newdata=testset)
    MSE[degree] <- mean((testset$mpg - ptest)^2)
  }
  data.frame(degree = 1:ndegrees, MSE = MSE)
}
```

Validation method on Auto

```r
validate(Auto,10)
```

```
##    degree      MSE
## 1       1 23.55361
## 2       2 17.16342
## 3       3 17.11455
## 4       4 17.48105
## 5       5 17.27775
## 6       6 18.69245
## 7       7 18.63700
## 8       8 18.98228
## 9       9 18.77249
## 10     10 19.08101
```

Problems with the validation method

- Splitting reduces the size of the sample used to fit the model.
- The tuning parameter that gives the best MSE can vary by split.

```
validate(Auto,10)
```

```
##    degree      MSE
## 1       1 26.61893
## 2       2 21.15002
## 3       3 21.11454
## 4       4 21.11325
## 5       5 20.45691
## 6       6 20.24181
## 7       7 20.03533
## 8       8 20.06858
## 9       9 20.46171
## 10     10 20.73248
```

Cross validation

- Split the data into k “folds”
  - Typical values of k are 5 and 10
- Leave out the first fold as a test set and train on the remaining folds.
- Repeat, leaving out each fold in turn.
- Report the average MSE over the folds.

Cross validation on the Auto data

```
createFolds <- function(n,k) { cut(1:n,breaks=k,labels=FALSE) }
crossValidate <- function(dat,ndegrees,k=10) {
  n <- nrow(dat)
  pdat <- dat[sample(1:n),]
  folds <- createFolds(n,k)
  MSE <- matrix(NA,nrow=ndegrees,ncol=k)
  for(degree in 1:ndegrees) {
    for(fold in 1:k) {
      trainset <- pdat[folds != fold,]
      testset <- pdat[folds == fold,]
      fit <- lm(mpg ~ poly(horsepower,degree),data=trainset)
      ptest <- predict(fit,newdata=testset)
      MSE[degree,fold] <- mean((testset$mpg - ptest)^2)
    }
  }
  data.frame(degree = 1:ndegrees, MSE = rowMeans(MSE))
}
```

Cross validation on Auto

```r
crossValidate(Auto,ndegrees=10)
```

```
##    degree      MSE
## 1       1 24.32184
## 2       2 19.19603
## 3       3 19.25960
## 4       4 19.28926
## 5       5 18.87781
## 6       6 18.79886
## 7       7 18.60278
## 8       8 18.81882
## 9       9 18.96773
## 10     10 19.14339
```

The caret package

- The caret package is supposed to contain many functions to help with training and fitting models.
    - Have never used it myself.